

# Scanning the Topological Sectors of the QCD Vacuum with Hybrid Monte Carlo

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We address a long standing issue and determine the decorrelation efficiency of the Hybrid Monte Carlo algorithm (HMC), for full QCD with Wilson fermions, with respect to vacuum topology. On the basis of five state-of-the art QCD vacuum field ensembles (with 3000 to 5000 trajectories each and  $\frac{m_\pi}{m_\rho}$ -ratios in the regime  $> 0.56$ , for two sea quark flavours) we are able to establish, for the first time, that HMC provides sufficient tunneling between the different topological sectors of QCD. This will have an important bearing on the prospect to determine, by lattice techniques, the topological susceptibility of the vacuum, and topology sensitive quantities like the spin content of the proton, or the  $\eta'$  mass.

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## I. INTRODUCTION

In the past, a reliable access to topological quantities of the QCD vacuum by methods of Lattice Gauge Theory has turned out to be a real challenge to the entire lattice approach.

Considerable progress has been achieved recently in the understanding of how to extract topological observables which are inherently continuum quantities from the discrete lattice. It was shown [1] that the field theoretical [2] and the geometrical [3] definitions of the topological charge yield—when suitably renormalized—equal values for the topological susceptibility,  $\chi$ , in the continuum. For practical purposes, however, we prefer the former

definition, as it offers superior quality of the stochastic signal [1].

This being settled, there remains the severe problem: any trustworthy stochastic sampling method must qualify to sufficiently decorrelate the members of the Monte Carlo time series with respect to the observables of interest; and the folklore is that the topological charge is the slowest of them all.

This nuisance is particularly aggravated in presence of dynamical fermions in QCD as they induce long range interactions, in form of the determinant of the fermionic matrix  $M$  inside the path-integral. Standard Hybrid Monte Carlo algorithms (HMC) deal with this non-local problem by recourse to a stochastic Gaussian representation of  $\det(M)$  [4]. Such treatment implies the repeated *costly* solution of large systems of linear equations which puts narrow limits on the affordable sample sizes, even on Teracomputers. Thus autocorrelations on the HMC time series are an issue of prime importance in judging the statistical reliability of estimates from HMC in realistic settings.

A failure of stochastic methods to scan the topological sectors of the QCD vacuum would be a real blow to lattice gauge theory, as topology is known to be of great importance to elementary particle physics: think of the Witten-Veneziano explanation of the  $\eta'$  mass, the relation of the axial vector current divergence to the topological charge density through the Adler-Bell-Jackiw anomaly, or the rôle of instantons in the structure of the vacuum.

For *staggered fermions*, indications have been given for quite insufficient tunneling rates of the topological charge

at very small mass parameters, both for two and four flavors [5,6].

Some of us [8] have performed simulations with four flavours of staggered fermions using the HMC. At  $\beta = 5.35$ , on a  $16^3 \times 24$  lattice, the time history exhibits little mobility, over 450 trajectories if the quark mass is chosen as  $ma = 0.01$  corresponding to  $\frac{m_\pi}{m_\rho} = 0.57(2)$ . Much shorter autocorrelation times, of the order of 10 trajectories, are found at  $ma = 0.02$  and  $ma = 0.05$ . These quark masses correspond to  $\frac{m_\pi}{m_\rho} = 0.65(3)$  and  $\frac{m_\pi}{m_\rho} = 0.75(1)$ .

For full QCD with dynamical *Wilson fermions* trustworthy results for the topological decorrelation efficiency of fermion algorithms are missing in the literature. In this note we report on an investigation that will fill this gap.

Our results are based on the high statistics samples as obtained by the SESAM [10] and T $\chi$ L [11] projects with HMC on APE100 hardware in Italy and Germany. The present sample consists of three time histories on lattices of size  $16^3 \times 32$  [12] at  $\kappa = 0.156, 0.157$ , and  $0.1575$ , corresponding to three intermediate  $\frac{m_\pi}{m_\rho}$  ratios of  $0.839(4)$ ,  $0.755(7)$ , and  $0.69(1)$ , respectively. At the coupling  $\beta = 5.6$ , the scale computed from the  $\rho$  mass is  $a^{-1} = 2.33(6)$  GeV [13], after chiral extrapolation. In the framework of the T $\chi$ L project, SESAM's set has been complemented by two ensembles of configurations on  $24^3 \times 40$  lattices, again at  $\beta = 5.6$ , with  $\kappa = 0.1575$  and  $0.158$ , the latter value corresponding to the lightest sea-quark mass attempted till now for Wilson fermions, with  $\frac{m_\pi}{m_\rho} = 0.56(2)$  [12].

So far, the SESAM sample has been partially analysed for integrated autocorrelation times of standard observables only, like plaquette, extended Wilson loops and octet hadron masses [14]. The autocorrelation time,  $\tau_{int}$  of these observables appears to be bounded by the one of the lowest eigenvalue of the Wilson fermion matrix, the bound being of size 15 to 30 in units of molecular dynamics time. In this sense, we can start with sets of about 200 such 'decorrelated' configurations to search for tunneling through the topological sectors.

## II. TWO WAYS TO MONITOR FOR TOPOLOGICAL CHARGE

The topological charge  $Q$  is the integral over space-time of the topological charge density,  $Q(x)$ , which is related via the  $U_A(1)$  anomaly of the flavor singlet axial current,  $\partial^\mu J_\mu^5(x) = 2N_f Q(x)$ .

To monitor for the topological content along the time histories, we use two independent methods to estimate  $Q$ :

1. The *gluonic* calculation, which starts from the charge density

$$Q(x) = \frac{g^2}{64\pi^2} \epsilon^{\mu\nu\rho\sigma} F_{\mu\nu}^a(x) F_{\rho\sigma}^a(x). \quad (1)$$

For the lattice definition of  $Q$  we follow Ref. [2]. Local fluctuations of the gauge fields are suppressed by the standard cooling procedure [7] just as in Ref. [8].

2. The *fermionic* evaluation follows the Smit and Vink proposal [9] which is inspired by the Atiyah-Singer theorem:

$$Q = m \kappa_P \langle \text{Tr}(\gamma_5 G) \rangle_U. \quad (2)$$

Here  $G$  represents the quark propagator in the background gauge field  $U$  with quark mass  $m$ .  $\kappa_P$  is a renormalization constant. No cooling is applied here.

We comment that both methods are in principle prone to characteristic systematic errors: while the gluonic approach might suffer from loss of instantons due to cooling, the fermionic monitor might be affected by 'dislocations'. It would therefore be gratifying to see them agree in their monitoring functionality.

To our knowledge, the Smit-Vink proposal has never been really exploited. Computing the trace in Eq. (2) requires the application of stochastic estimator techniques. Such estimates in general turn out to be extremely noisy. However, thanks to recent progress in noise reduction methods achieved by some of us [15], we are now in the position to extract rather accurate signals for  $\text{Tr}(\gamma_5 G)$ .

## III. RESULTS

With the procedures described in the previous section we are sufficiently equipped to monitor for the decorrelation of the topological charge in the HMC process.

Fig. (1) shows the time series for  $Q$  as measured on our ensembles. The first three graphs contain 200 configurations each. These ensembles were taken from contiguous series of trajectories of length 5000, produced by SESAM on  $16^3 \times 32$  lattices. The configurations are separated by 25 units in absolute molecular dynamics time. In the first three graphs, the results from the gluonic and fermionic measurements are super-imposed. We find them to agree nicely which demonstrates that the systematic errors of both methods are sufficiently under control.

First inspection shows many tunneling events of the topological charge between the distinct sectors, for all three sea quark masses on the  $16^3 \times 32$  lattices. There seems to be a tendency that the fluctuations decrease with increasing  $\kappa$ . In an attempt to quantify these features we introduce the mobility of tunneling,  $D_d$ , as the average weighted number of tunneling events measured on configurations which are separated by a distance of  $d$  along the time history:

$$D_d = \frac{1}{N-1} \sum_{i=1}^{N-1} |(\tilde{Q}(i+1) - \tilde{Q}(i))|, \quad (3)$$

with  $\tilde{Q}$  being the integer value of the measured quantity  $Q$  and  $N$  the number of measurements. The resulting numbers are given in table I. They reflect the tunneling rates and thus the decorrelation capability of HMC, when approaching the chiral limit.

It should be noted, however, that  $D_d$  depends on the volume for two reasons:  $D_d$  has not been normalised to the amplitude of the fluctuations and our HMC parameters have been retuned when the system size was changed.

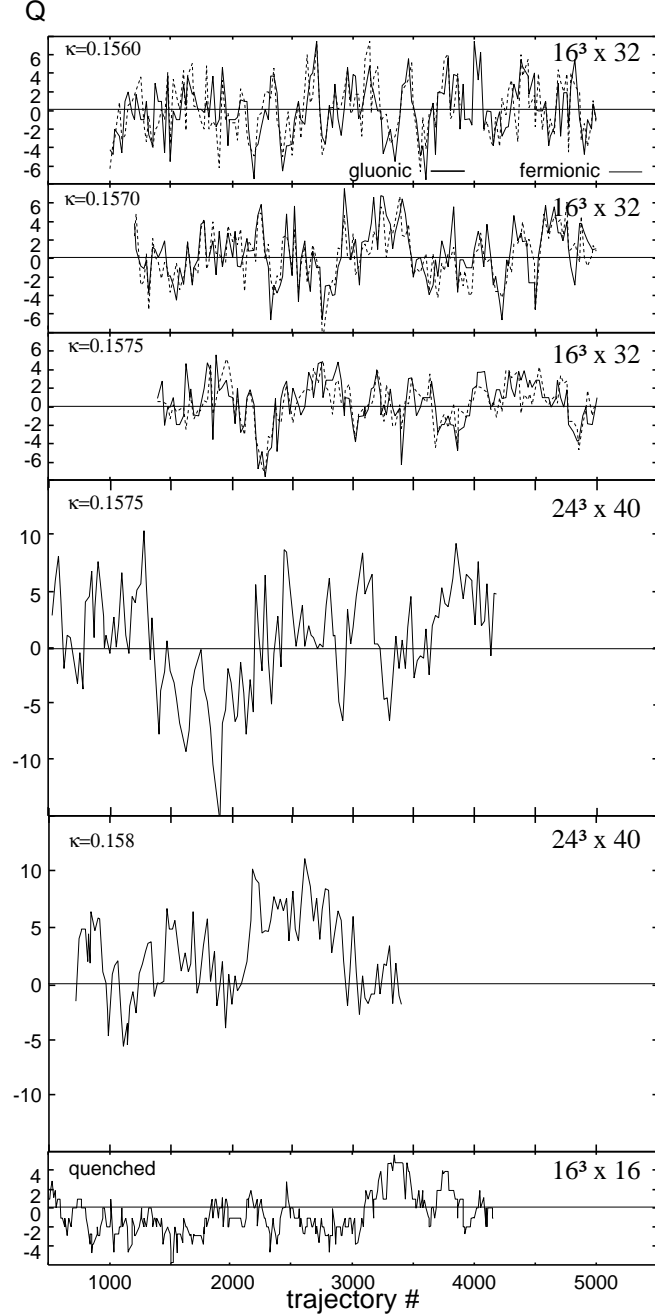


FIG. 1. Time series of topological charge. We plot series from 3 SESAM and 2 T $\chi$ L ensembles. The last canvas is a quenched HMC simulation at  $\beta = 6.0$ .

With the entire time histories of our HMC runs being archived we are able to postprocess all trajectories from the SESAM and T $\chi$ L samples. For  $\kappa = 0.1575$ —the smallest SESAM mass—we have computed the topological charge on a contiguous segment of  $> 5000$  trajectories for every second trajectory, see Fig. (2). We find the topological charge to change frequently on that time scale. This is illustrated in the zoom of Fig. (2), which shows considerable fluctuations on that time scale.

The series for  $\kappa = 0.1575$  is long enough to allow for the computation of the autocorrelation function, as plotted in Fig. (3). We can apply an exponential fit to its ‘slowest’ mode. The fit reveals the exponential autocorrelation time of  $\tau_{exp} = 80(10)$ . The integrated autocorrelation time from the lower diagram in Fig. (3) turns out to be  $\tau_{int} = 54(4)$ . These numbers should be compared to the upper bound of  $\tau_{int}$  as estimated from other observables,  $\max \tau_{int} = 42(4)$  [14].

The tunneling behaviour is reflected in the histograms of Fig. (4). The errors quoted have been estimated by naive jackknife. The distributions are well peaked at  $Q = 0$ . With 200 entries, though, the symmetry is not yet so well established.

Histogramming the fine scan of Fig. (2), we arrive at the fourth histogram which comprises 2500 entries. We find a smooth Gaussian shape to emerge, see Fig. (4).

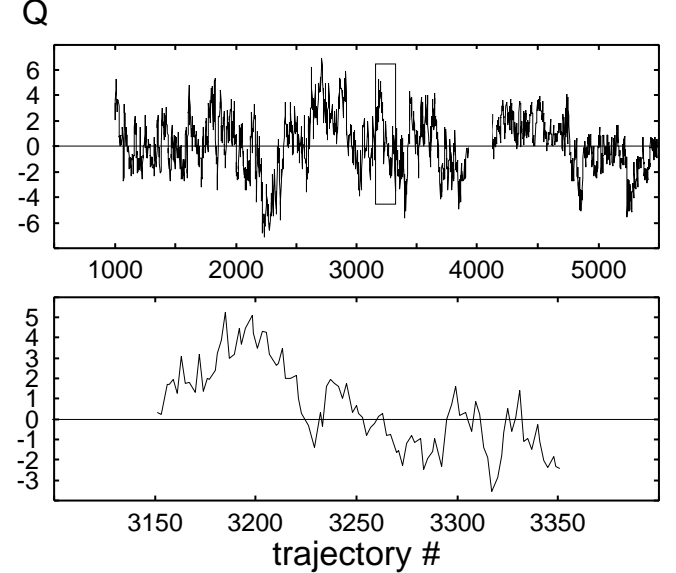


FIG. 2. Fine scan of  $Q$  for  $\kappa = 0.1575$  on the  $16^3 \times 32$  lattice. The second canvas is a zoom.

Finally, we turn to the volume dependency. On the  $24^3 \times 40$  system, at  $\kappa = 0.1575$ , the time history looks rather much alike to the one on the  $16^3 \times 32$  lattice, apart from an apparent increase in amplitude. The mobility at a separation of 25 units of molecular dynamics time,  $D_{25}$ , turns out to be twice as large as for the small system, see table I. Naively, we would expect that the mobility scales approximately with the square root of the volume,

leading to a factor of two. However, we remark that on the large system, we had to re-adjust the length of the molecular dynamics trajectory to  $T = 0.5$ . Thus, for the chosen separation of  $T = 25$ , we refresh momenta and fermions twice as often as on the smaller system.

Going more chiral, at  $\kappa = 0.1580$ , our present sample size is not sufficient to make definite statements, as the expected symmetry around  $\langle Q \rangle = 0$  is not yet established.

The last entry in Fig. (1) refers to a HMC series in the quenched case at  $\beta = 6.0$ , on a  $16^4$  lattice. The reduced volume amounts to a smaller amplitude. The series appears to be less ergodic on the time scale of 4000 trajectories, compared to the three full-QCD runs on the  $16^3 \times 32$  lattice. The mobility in the quenched case is observed to take the value 1.2.

#### IV. DISCUSSION AND OUTLOOK

We find that HMC is capable to create sufficient tunneling between the vacuum sectors when dealing with dynamical Wilson fermions for  $\frac{m_\pi}{m_\rho} > 0.56$ .

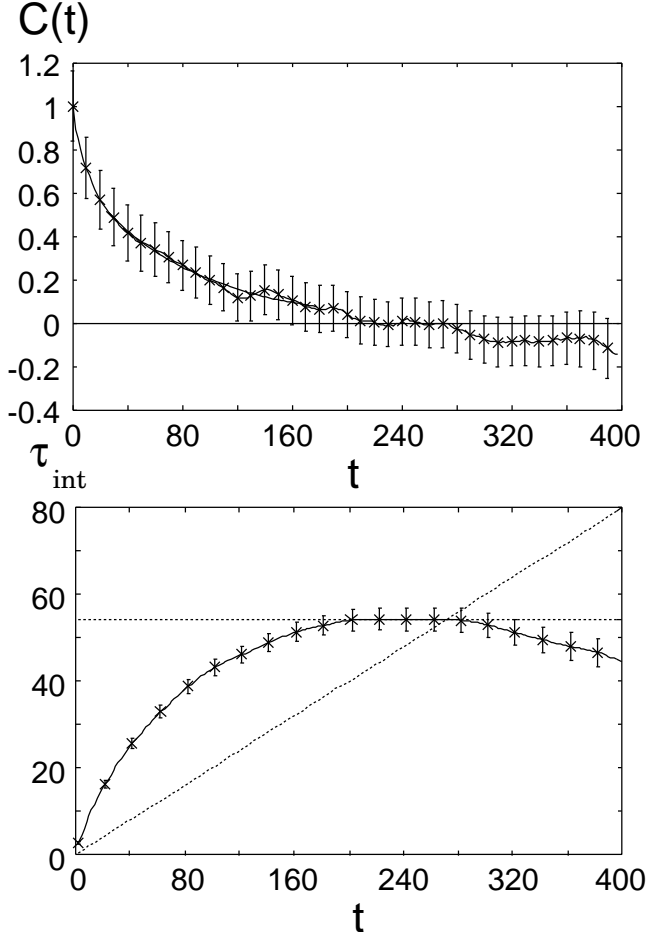


FIG. 3. Autocorrelation function and integrated autocorrelation time of  $Q$  for  $\kappa = 0.1575$  on the  $16^3 \times 32$  system.

This is seen with both, gluonic and fermionic determinations of  $Q$  which proves their reliability as monitoring devices.

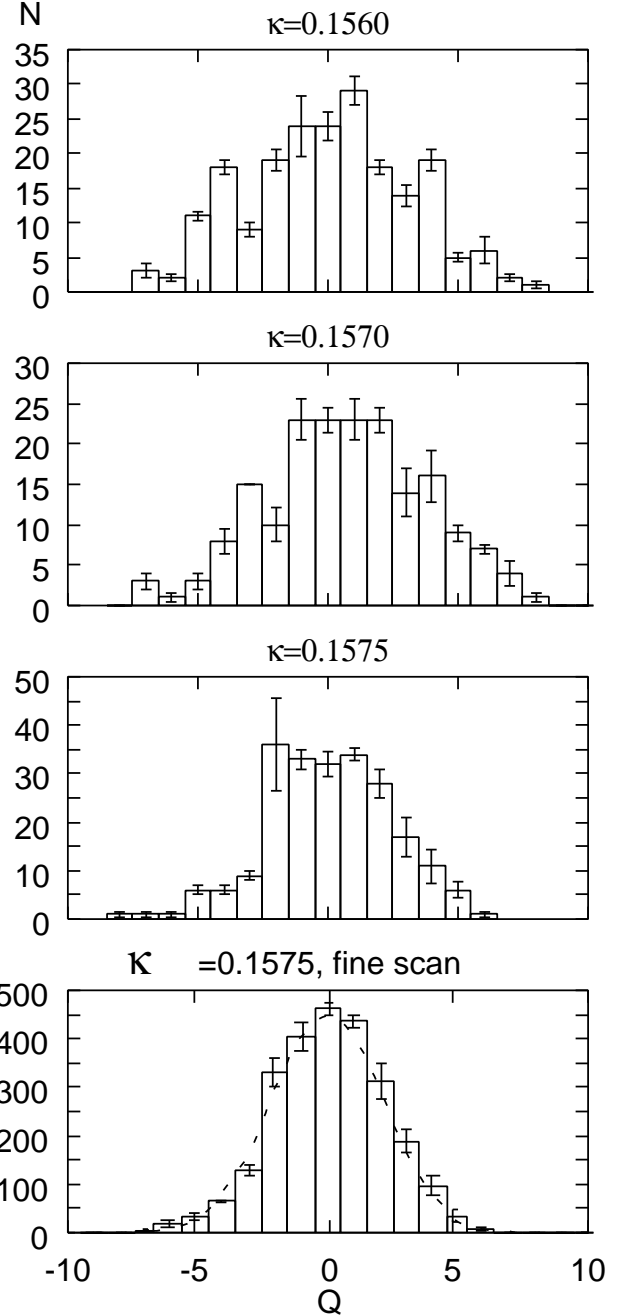


FIG. 4. Histograms of the topological charge.

TABLE I. Mobility  $D_{25}$ , see eq. 3.

$\kappa$	0.1560	0.1570	0.1575	0.1580
$16^3 \times 32$	2.8	2.5	1.9	-
$24^3 \times 40$	-	-	3.8	2.8

The autocorrelation rates as determined from various non-topological quantities are in accord with the autocorrelation time of the topological charge. It is interesting to note that the high frequency mobility of HMC with respect to topology is important for achieving the expected symmetry of the topological charge distributions.

When approaching the chiral regime, at  $\kappa = 0.1580$  or  $\frac{m_\pi}{m_\rho} = 0.56$ , we would expect to need a sample size of order 10.000 to achieve sufficient ergodicity with respect to topology. This is definitely in the reach of teracomputing.

It is evident that the fermionic force plays an important rôle for the tunneling efficiency of HMC: in the quenched setting, HMC appears to be less efficient in driving the system through the topological sectors. In order to understand this effect in more detail further studies are needed.

At this point, with the available sample, we are in the position to study hadronic properties related to topology, like the proton spin content and the topological susceptibility for  $\frac{m_\pi}{m_\rho}$ -values down to 0.69. Work along this line is in progress.

Another line of research being followed by some of us [16] is the tunneling efficiency of alternative stochastic algorithms, such as the multibosonic method [17].

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